FILTERED DENSITY FUNCTION FOR SUBGRID SCALE MODELING OF TURBULENT DIFFUSION FLAMES

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SUMMARY/OVERVIEW:

Within the past year, our work was concentrated primarily on three issues: (1) further development and improvements of the joint velocity-scalar filtered mass density function (VSFMDF) as a subgrid scale (SGS) closure, (2) finalizing the implementation of the scalar filtered mass density function (SFMDF) for large eddy simulation (LES) of a turbulent bluff-body flame, and (3) improvement of the computational efficiency of our FDF codes.

TECHNICAL DISCUSSION:

This research is focused on development and implementation of the filtered density function (FDF) method for subgrid scale (SGS) closure of turbulent combustion. Within the past few years, the FDF methodology has become very popular; see Givi [1] for a recent review. In addition to our previous AFOSR-sponsored work [2–6], the methodology has experienced widespread usage by many others. Examples are contributions in its basic implementations [7, 8], fine-tuning of its sub-closures [9–11], and its validation via laboratory experiments [12–15]. The methodology is finding its way into commercial codes such as Fluent, and has been the subject of detailed discussions in several recent textbooks [16–18].

The latest development in, and up to now the most comprehensive means of, the FDF formulation is via the joint velocity-scalar filtered mass density function (VSFMDF). Within the past year, we have fine-tuned the physical modeling and the computational procedure of the VSFMDF. Simulations were conducted of a three-dimensional temporally developing, variable density mixing layer involving transport of a passive scalar. Direct numerical simulation (DNS) was conducted of this flow, and comparisons were also made with LES via the Smagorinsky model. Various effects of density variations [19] are investigated. The results of this study are discussed in detail in a recent Ph.D. dissertation [20]. Some sample results are presented here. Figure 1 shows the filtered fluid density field for several values of the free-stream density ratios of s. As shown, there are good agreements between VSFMDF and DNS. As the density ratio increases, the shear layer center is shifted further to the low-density side. As a result, the peak values of the Reynolds stresses and scalar fluxes also shift

to the low-density side. This shift is responsible for the reduction of the turbulent production terms [19], and thus the decrease of the shear layer thickness [21]. The temporal variation of the "scalar thickness" is presented in Fig. 2. The Smagorinsky model underpredicts the spread of the layer due to its dissipative nature. All VSFMDF predictions compare well with DNS data.

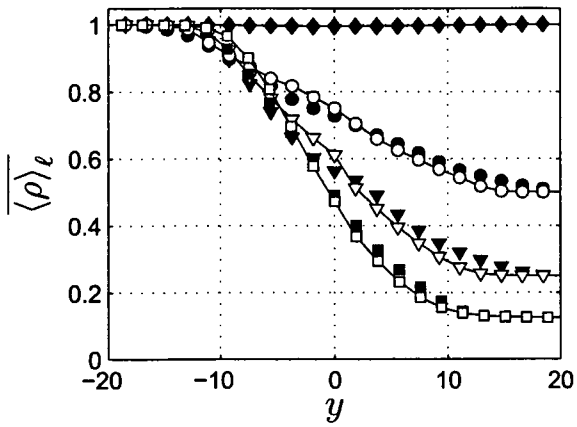

FIGURE 1: Cross-stream variation of Reynolds-averaged density in temporal mixing layer simulations. The solid lines with open symbols denote VSFMDF predictions. The filled symbols denote DNS data. The symbols denote: (diamond) $s = 1$, (circle) $s = 2$, (triangle) $s = 4$, and (square) $s = 8$.

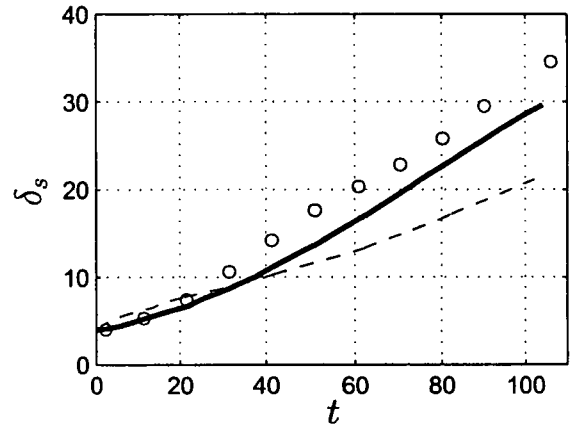

FIGURE 2: Temporal variation of scalar thickness in temporal mixing layer simulations with $s = 2$. The thick solid and thin dashed lines denote LES predictions using VSFMDF and Smagorinsky closures, respectively. The white and black circles show the filtered and unfiltered DNS data, respectively.

After our successful prediction of the piloted jet flame [2], we applied our scalar filtered mass density function (SFMDF) methodology for LES of the University of Sydney bluff-body flame [22–24]. This part of our work is described in detail in a recent Ph.D. dissertation [25]. Some sample results are shown here. The time averaged streamwise velocity contours with the streamlines and velocity vectors superimposed are shown in Fig. 3. This figure shows the recirculation region and the two characteristic counter-rotating vortices. The recirculating zones are captured well by the simulations. The comparisons also show good overall qualitative agreement with data. The quantitative agreement with data is also very good for the mean, rms values, and PDFs of various fields (see Fig. 4). Our previous work on application of the FDF to complex flames suggest that in order to apply this methodology to more realistic geometries with realistic reaction models, the hybrid finite-difference (FD)/Monte Carlo (MC) numerical solution procedure needs to be more-effectively parallelized. This allows us to take advantage of more computational power and large number of processor in FDF simulations. Therefore, within the past year, a part of our effort was devoted to improving the parallel efficiency of our FDF codes. The parallelization is implemented by dividing the computational domain into equal-sized sub-domains. Each processor performs the FD procedure separately on each of these domains. The message-passing interface (MPI) library is used to pass the variables between processors. This implementation ensures load balancing. The message-passing is implemented in a non-blocking manner,

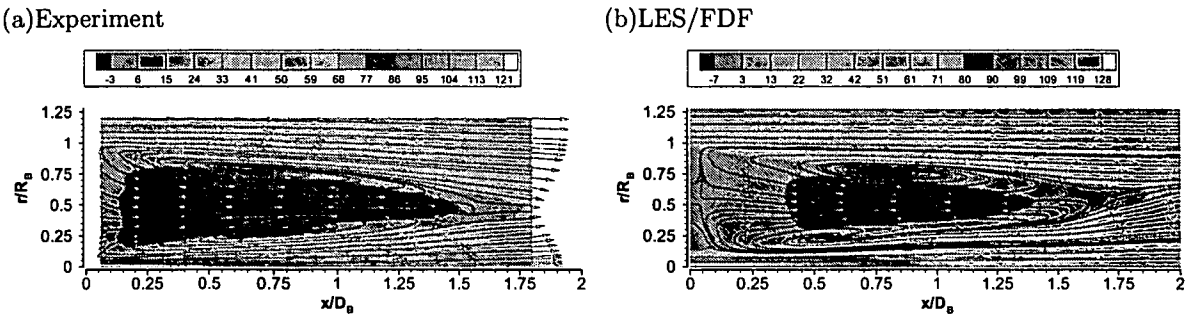

FIGURE 3: Time averaged recirculation features as predicted by FDF. The contours denote the streamwise velocity. Superimposed are the streamlines and the velocity vectors.

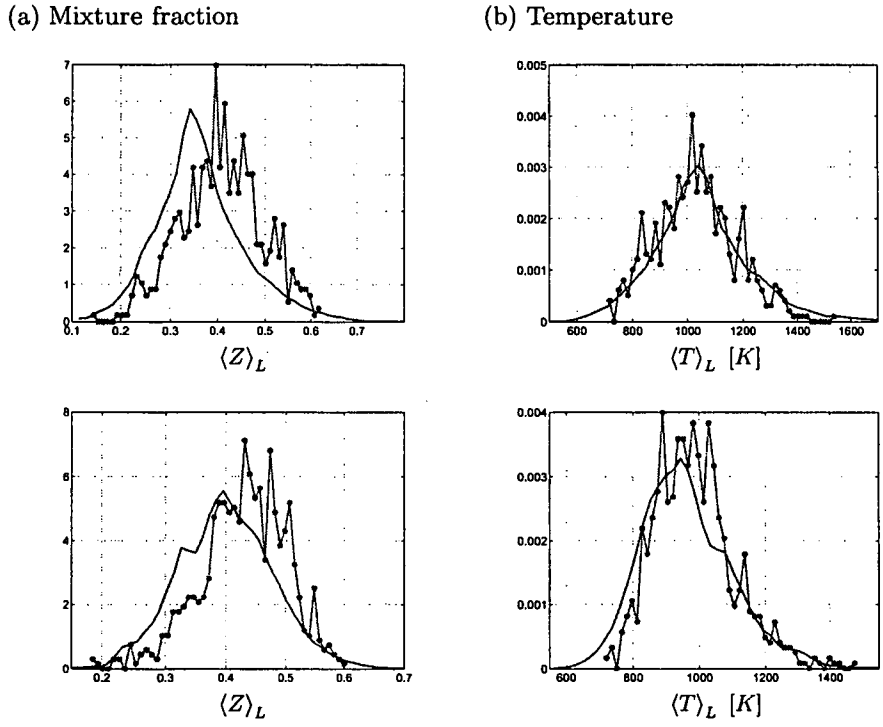

FIGURE 4: PDFs of the resolved (a) mixture fraction, and (b) temperature at the radial location $r = 5.05\ mm$ compared to the experiment. (top-to-bottom rows) $x/D_B = 0.9$, and 1.3. —— FDF, —●— Experiment.

to enable overlapping of communications with computations. This results in reduction of communication overhead. The parallelization of MC procedure is done by dividing the MC particles among the processors according to their spatial location. This way the particles have direct access to FD variable they need for their evolution. Each MC particle evolves independently, thus there is no inter-particle interactions. As the particles move, they may translate to the neighboring sub-domain. This is done by communicating the particle values between the adjacent processors. Due to random stochastic nature of particle motion, there is a substantial increase in communication overhead due to particle oscillation near the

sub-domain's boundaries. To alleviate this, a buffer zone is devised in which the particles are accumulated. With this treatment, the particle communications are not needed at each time step and the communication overhead is decreased significantly. The procedure as developed here is examined extensively on up to 64 processors. The results show good load balancing and close to linear speed-ups.

ACKNOWLEDGEMENTS:

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